

CNRS - Université Pierre et Marie Curie - Université Versailles-Saint-Quentin  
CEA - ORSTOM - Ecole Normale Supérieure - Ecole Polytechnique



# Institut Pierre Simon Laplace

## des Sciences de l'Environnement Global

# OPA 8.1 Tracer Model Reference Manual

Marie-Alice Foujols\*, Marina Lévy\*\*,  
Olivier Aumont\*\*\*,‡, and Gurvan Madec\*\*

\* *Institut Pierre Simon Laplace*

\*\* *Laboratoire d'Océanographie DYnamique et de Climatologie*

‡ *previously at Laboratoire des Science du Climat et de l'Environnement*



**July 2000**



# OPA 8.1 TRACER MODEL

## REFERENCE MANUAL

Marie-Alice Foujols\*, Marina Lévy\*\*,  
Olivier Aumont\*\*,<sup>‡</sup> and Gervan Madec\*\*

\* Institut Pierre Simon Laplace, Paris, France  
(CNRS/UPMC/UVSQ/CEA/IRD/ENS/EP)

\*\* Laboratoire d'Océanographie Dynamique et de Climatologie, Paris, France  
(CNRS/IRD/UPMC)

<sup>‡</sup> previously at Laboratoire des Sciences du Climat et de l'Environnement, Gif-sur-Yvette, France  
(CEA/CNRS)

[mafoipsl@ipsl.jussieu.fr](mailto:mafoipsl@ipsl.jussieu.fr)

[marina.levy@ipsl.jussieu.fr](mailto:marina.levy@ipsl.jussieu.fr)

[aumont@lsce.saclay.cea.fr](mailto:aumont@lsce.saclay.cea.fr)

[madec@lodyc.jussieu.fr](mailto:madec@lodyc.jussieu.fr)



<b>INTRODUCTION.....</b>	<b>1</b>
<b>I. MODEL BASICS.....</b>	<b>3</b>
<b>II. NUMERICAL RESOLUTION.....</b>	<b>5</b>
<i>II.1 SMS terms.....</i>	<i>5</i>
<i>II.2 Advection.....</i>	<i>5</i>
<i>II.3 Vertical diffusion.....</i>	<i>6</i>
<i>II.5 Lateral diffusion.....</i>	<i>6</i>
<i>II.6 Global temporal resolution.....</i>	<i>7</i>
<b>III. DETAILS OF THE CODE .....</b>	<b>9</b>
<i>III.1 Code architecture.....</i>	<i>9</i>
<i>III-3 Flow chart.....</i>	<i>12</i>
<i>III-3 Parameters.....</i>	<i>13</i>
<i>III-4 Namelist.....</i>	<i>13</i>
<i>III-5 Performances.....</i>	<i>14</i>
<b>IV. SPECIFICITIES OF THE OFFLINE CODE .....</b>	<b>17</b>
<i>VI-1 Generalities.....</i>	<i>17</i>
<i>VI-2 Flow chart.....</i>	<i>17</i>
<i>VI-3 Specific off-line options.....</i>	<i>17</i>
<b>APPENDIX A : THE ADVECTION SCHEMES .....</b>	<b>19</b>
<i>A-1 Arakawa and Smolarkiewicz advection schemes.....</i>	<i>19</i>
<i>A-2 Associated temporal schemes.....</i>	<i>21</i>
<i>A-3 Numerical cost.....</i>	<i>22</i>
<b>APPENDIX B : THE NPZD BIOGEOCHEMICAL MODEL .....</b>	<b>23</b>
<i>B-1 The surface layer NPZD model.....</i>	<i>23</i>
<i>B-2 The optical model.....</i>	<i>24</i>
<i>B-3 Remineralization.....</i>	<i>26</i>
<b>APPENDIX C : THE NNPZDDOM BIOGEOCHEMICAL MODEL .....</b>	<b>27</b>
<i>C-1 The surface layer NNPZDDOM model.....</i>	<i>27</i>
<i>C-2 The optical model.....</i>	<i>29</i>
<i>C-3 Remineralization.....</i>	<i>29</i>
<b>APPENDIX D : THE HAMOCC3 BIOCHEMICAL MODEL.....</b>	<b>31</b>
<i>D-1 The surface layer biological production.....</i>	<i>31</i>
<i>D-2 Export and Remineralization.....</i>	<i>32</i>
<i>D-3 Gas exchange.....</i>	<i>33</i>
<b>APPENDIX E : THE P3ZD BIOCHEMICAL MODEL .....</b>	<b>35</b>
<i>E-1 The surface layer P3ZD model.....</i>	<i>35</i>
<i>E-2 The optical model.....</i>	<i>37</i>
<i>E-3 Remineralization.....</i>	<i>38</i>
<i>E-4 Carbon and silicon cycles.....</i>	<i>39</i>



## INTRODUCTION

The tracer transport model implemented in OPA deals with passive tracers, which are transported by but do not affect ocean circulation. These contrast with active tracers such as temperature and salinity that feedback on ocean dynamics.

The tracer transport model computes the evolution of passive tracers either “on-line” along with the dynamics, or “off-line“ using fields of advection and diffusion that have been previously calculated and stored to disk.

Passive tracers in the ocean are typically biogeochemical, biological or radioactive. They are transported by the oceanic circulation, but they may in nature also degrade or interact with one another. Typically, the associated "Source-Minus-Sink" (SMS) terms are also included in the transport equation and depend upon the application.





## I. MODEL BASICS

Passive tracers follow the transport equation, forced with specific SMS terms. The transport equation of a passive tracer  $C$  is similar to that of temperature (see OPA reference manual, §I-3 and §I-5 for notations):

$$\frac{\partial C}{\partial t} = S(C) - \left[ \frac{1}{e_1 e_2} \left( \frac{\partial(e_2 C u)}{\partial i} + \frac{\partial(e_1 C v)}{\partial j} \right) + \frac{1}{e_3} \frac{\partial(C w)}{\partial k} \right] + D^{lC} + D^{vC} \quad (1)$$

where expressions of  $D^{lC}$  and  $D^{vC}$  depend on the choice for the lateral and vertical subgrid scale parameterizations.

$S$ , the first term on the right hand side of (1), is the SMS term inherent to the tracer. In the case of a biological tracer such as phytoplankton,  $S$  is the balance between phytoplankton growth and its decay through mortality and grazing. In the case of a radioactive tracer,  $S$  is simply loss due to radioactive decay.

The second term (within brackets) represents the advection of the tracer in the three directions. It can be interpreted as the budget between the incoming and outgoing tracer fluxes in a volume element  $b = e_1 e_2 e_3$ .

The third term in equation (1) represents the change due to lateral diffusion. In OPA, four options for lateral mixing are offered for *active* tracers in the  $z$ -coordinate formulation:

- second-order geopotential operator (laplacian)
- second-order isopycnal operator
- Gent and McWilliams (1990) parameterization
- fourth-order geopotential operator (biharmonic)

In the  $s$ -coordinate formulation, a second order operator acting along  $s$ -surfaces is also available (see OPA reference manual §I-5). In the tracer model, lateral diffusion of passive tracers is compulsory. When activated, lateral diffusion works in the same way as for active

tracers and uses the same value of the lateral eddy diffusivity. The  $s$ -coordinate formulation is not yet implemented.

The fourth term is change due to vertical diffusion, parameterized as eddy diffusion to represent vertical turbulent fluxes:

$$D^{vC} = \frac{1}{e_3} \frac{\partial}{\partial k} \left( \frac{1}{e_3} A^{vT} \frac{\partial C}{\partial k} \right) \quad (2)$$

where  $A^{vT}$  is the vertical eddy diffusivity coefficient of *active* tracers. Several options exist to specify vertical diffusion of active (and passive) tracers: constant value, Richardson number dependent value, 1.5 turbulent closure scheme, enhanced vertical diffusion. These options are fully described in the OPA reference manual (§III-7). However, the non-penetrative convective adjustment algorithm that is sometimes used for active tracers has not been implemented for passive tracers.

## II. NUMERICAL RESOLUTION

The tracer transport equation is discretized on the same grid as the other variables of the OPA code, with passive tracers located at the center of each grid cell, *i.e.* at active tracer points (*T*-points). The reader is referred to the OPA reference manual §II for complete information about the discretization and the grid. The integration method is the same as that used for active tracers: each term of the right hand side of the equation is computed separately, with a specific spatial and temporal scheme, then all components are combined during time integration.

### II.1 SMS terms

The SMS terms are usually complicated functions of tracer concentrations. They are computed explicitly from concentrations taken at the previous time step (*i.e.* a backward temporal scheme is used). Four different SMS models are provided as examples in Appendix B to E.

### II.2 Advection

In OPA, the advection of active tracers is resolved numerically with a centered-in-space scheme, known as the “leapfrog” scheme (Messinger and Arakawa, 1976). The leapfrog scheme is conservative and non-dissipative (*i.e.* it conserves the variance), but it presents two main shortcomings: it is non-steady and can lead to the apparition of anomalous tracer

minima and maxima. It is not adapted for computation of advection of passive tracers, which fields are often close to zero and require positive definite schemes. The *Flux Corrected Transport* (FCT) method of Smolarkiewicz (1986) fulfils this need. It is a conservative but slightly diffusive scheme, which conserves with good accuracy the maxima of the transported field. The FCT method can only be used with tracers having positive values everywhere. The choice between the Arakawa and FCT schemes is left to the user. Both spatial schemes and their associated temporal schemes are detailed in Appendix A.

Additional positive definite advective schemes are currently being tested and should be available in the next release.

### **II.3 Vertical diffusion**

For stability, vertical diffusion is treated implicitly with a forward time scheme. Vertical diffusion is computed last because implicit computation requires all other terms in the equation. The scheme is identical to that used for temperature (see OPA reference manual §II-2c). Note that in OPA there is an option to explicitly integrate vertical diffusion. This option is not available for passive tracers.

### **II.5 Lateral diffusion**

Lateral diffusion is discretized in the same way for passive tracers as it is for active tracers (see OPA reference manual §II-2c), with a forward temporal scheme. The user should be aware that biharmonic operator does not insure the conservation of positivity, contrary to laplacian one. However there is also the possibility not to use any explicit lateral diffusion ; such an option is recommended when using the FCT scheme in eddy-resolving configurations, as the diffusion inherent to the FCT scheme might be sufficient to insure numerical stability.

## II.6 Global temporal resolution

The global temporal resolution is dictated by the choice of the advective scheme. When the Arakawa scheme is used, temporal integration is achieved with a leapfrog scheme associated with a Robert-Asselin time filter. On the other hand, the FCT scheme requires a forward time integration, with velocity fields centered in time. For that reason, the use of FCT implies the time step for the passive tracers to be at least twice the time step for the dynamics (or a multiple of two dynamical time steps).



## III. DETAILS OF THE CODE

### III.1 Code architecture

#### 1. Generalities

The tracer model is automatically added to the OPA model if required during the execution of the `fait_make` (for the on-line version) or the `fait_make_offline` (for the off-line version) script.

It follows OPA's rules (see OPA 8.1 Ocean General Circulation Model - Reference manual - chapter IV-1). In particular, several options are available that can be set by defining tracer specific ***cpp keys*** (in bold italic). The user should be aware that some general OPA *cpp keys* (in italic) are also in use in the tracer module. This implies that the tracer code depends on the dynamical code. This will be further explained.

The tracer model consists in a series of additional files in a specific passive tracer directory (`LODMODEL/SRC_TRC_ORCA_SMS`), which are activated when the `cpp key` ***key\_passivetr*** is declared:

- `common.passivetr.h` : common statements for passive tracers.
- `parameter.passivetr.h` : specific parameters for passive tracers (see III-3)
- `namelist.passivetr` : general namelist for passive tracers (see III-4)
- `initrc.F` : entry point for initialization routines.
- `trc*.F`: besides `initrc`, all tracer routines (transport, inputs, outputs) begin with `trc`

There are four entry points in OPA for the passive tracer model: `initrc`, `trcstp`, `trcdia`, and `trcwri` (see flow chart III-3).

By default, two passive tracers are declared and are initialized with current *now* temperature and salinity fields. There are no SMS terms. Results should be the same as for the *T* and *S* active tracers if the following options are set: no penetrative heat flux (`key_fluxsr`

not declared), Arakawa advection scheme (*key\_trc\_arakawa*), lateral diffusion (*lhdf=.true.*), on-line code, same time step for active and passive tracers (*ndttrc=1*).

## 2. SMS options

### a) NPZD and NNPZDDOM models

If either *key\_trc\_npzd* or *key\_trc\_nnpzddom* is declared, the NPZD (resp. NNPZDDOM) model is invoked. This activates a certain number of additional routines and includes a certain number of *\*.npzd.h* (*\*.nnpzddom.h*, resp.) files, which can be found in the directory: [LODMODEL/SRC\\_TRC\\_ORCA\\_SMS/trc\\_sms](#).

- [common.passivetrn.npzd.h](#) : specific common statements for NPZD model.
- [parameter.passivetrn.npzd.h](#) : (forces *jptra = 4*)
- [namelist.sms.npzd](#) : specific namelist for NPZD model
- [trcbio.F](#), [trcbio.npzd.h](#), [trcopt.F](#), [trcsed.F](#) : specific routines for NPZD model
- [trcdib.h](#) : outputs of biological trends
- [trcini.npzd.h](#) : specific initialization for NPZD model
- [trclsm.npzd.h](#) : reads namelist for NPZD model
- [trcctl.npzd.h](#) : control options for NPZD model (in particular, forces the tracer names)

We suggest that if the user wants to define his own SMS model, he should follow these general construction and grep for *key\_trc\_npzd* in the source passive tracers directory.

### b) HAMOCC3 and P3ZD

If *key\_trc\_hamocc3* is declared, the HAMOCC3 model is invoked. A certain number of routines are then activated with some *\*hamocc3.h* files. All these files can be found in the directory: [LODMODEL/SRC\\_TRC\\_ORCA\\_SMS/trc\\_sms](#).

- [common.passivetrn.hamocc3.h](#) : specific common statements for HAMOCC3 model.
- [parameter.passivetrn.hamocc3.h](#) : (in particular *jptra = 7*)
- [namelist.sms.hamocc3](#) : specific namelist for HAMOCC3 model
- [h3cbio.F](#), [h3cche.F](#), [h3cexp.F](#), [h3cflux.F](#), [h3cice.F](#), [h3cint.F](#), [h3clys.F](#), [h3copt.F](#), [h3cprg.F](#), [h3crem.F](#), [h3crem.F](#), [h3cvfl.F](#), and [h3cwin.F](#): specific routines for HAMOCC3 model
- [trcdib.h](#) : outputs of biological trends
- [trcini.hamocc3.h](#) : specific initialization for HAMOCC3 model



□ `trclsm.hamocc3.h` : reads namelist for HAMOCC3 model

□ `trcctl.hamocc3.h` : control options for HAMOCC3 model (in particular, forces the tracer names)

To invoke the P3ZD model, both `key_trc_hamocc3` and `key_trc_p3zd` should be declared. P3ZD needs most routines from HAMOCC3, especially for the carbon chemistry and the air-sea gas exchange. Routines which are specific of P3ZD begin with the `p3z` letters. Basically these routines are `p3zbio.F` (biological production in the euphotic zone) and `p3zrem.F` (reminerzalization of organic matter below the euphotic depth). They respectively replace `h3cbio.F` and `h3crem.F`.

### 3. Dynamical options

□ **Coordinates:** the vertical coordinate system is necessarily that of the dynamics,  $z$ -coordinates by default,  $s$ -coordinate when the key `key_s_coord` is defined.

□ **Advection:** `key_trc_arakawa` must be defined in order to use the Arakawa advection scheme (Smolarkiewicz scheme is used by default).

□ **Diffusion:** the passive tracer diffusion has necessarily the same form as the active tracer diffusion. The choice relies on the defining of the following keys : `key_trahdfbilap`, `key_trahdfcoef1d`, `key_trahdfcoef2d`, `key_trahdfcoef3d`, `key_trahdfeiv`, `key_trahdfgeop`, `key_trahdfiso`. However, unlike for the dynamics, it is possible to run the tracer model without explicit horizontal diffusion by setting the logical parameter `lhdf` to false in the passive tracer namelist. Also, when using isopycnal diffusion, a different background coefficient can be used for the passive tracers, `ahtrb0`.

□ **Damping:** `key_trcdmp` (not fully implemented).

### 4. Diagnostics options

□ `key_trc_diatrd`: storage of dynamical trends (3 for advection, 3 for diffusion, 3 for eddy-induced advection if `key_trahdfeiv` is also defined). The array `trtrd(jpi,jpj,jpk,jptrajpdia3d)`, in which the trends are saved, is declared in the common. This highly increases the memory used. Arrays are saved at the frequency `nwrite3d` (namelist).

□ `key_trc_diaadd` : storage of additional 2-D or 3-D arrays. Enables for instance to save the sea surface concentration of a tracer with a higher output frequency (`nwriteadd` in the namelist). Additional arrays are `trc3d(jpi,jpj,jpk,jpdia3d)` and `trc2d(jpi,jpj,jpdia2d)`.

□ `key_trc_diabio` : enables the storage of biological trends (when `key_trc_npzd` or `key_trc_nnpzddom` is declared), `trcbio(jpi,jpj,jpk,jpdia3d)`, at the frequency `nwritebio`

□ `key_diainstant` : instantaneous output fields (averaged fields by default)

□ By default, outputs are in NETCDF format (GDT convention) using IOIPSL library (see also [www.ipsl.jussieu.fr/~ioipsl](http://www.ipsl.jussieu.fr/~ioipsl)). It is possible to output binary file (direct access file) by defining the CPP key *key\_fdir*.

### 5. Portability options

□ *key\_mpp* : must be defined for massively parallel processors (MPP).

□ *key\_mpp\_mpi* : must be defined for massively parallel processors (MPP) with MPI communication technique.

□ *key\_mpp\_shmem* : must be defined for massively parallel processors (MPP) with SHMEM technique like SGI-Cray T3E.

## III-3 Flow chart

Routines are sorted by call order. Routines in *italic* are standard OPA8 routines. Routines in **bold** are specific to the tracer module. Routines in **bold italics** are specific to examples in the SMS module.

<b>On-line passive tracer module flow chart</b>		
<i>modele</i>		Ocean General Circulation Model
<i>opa</i>	<b>initrc</b>	Initialization
	<b>trlec</b>	Reads namelist.passivetr
	<b>trclsm</b>	Reads namelist for SMS
	<b>trctl</b>	Controls the coherence of options
	<b>trcini</b>	Initializes all fields to zero
	<b>trcrst</b>	Initialization in case of restart
	<b>trcdtr</b>	Initialization : analytic or from file
<i>step</i>	<b>trcstp</b>	General time step loop
	<b>trcsms</b>	Passive tracers time step loop
	<b>trcopt</b>	Entry point for SMS routines
	<b>trcbio</b>	Optics (example)
	<b>trcsed</b>	Biology (example)
	<b>trchad</b>	Sedimentation (example)
	<b>trczad</b>	Horizontal advection (for Arakawa scheme)
	<b>trc3ad</b>	Vertical advection (for Arakawa scheme)
	<b>trchdf</b>	3D advection (for Smolarkiewicz scheme)
	<b>trcsbc</b>	Horizontal diffusion (if required)
	<b>trczdf</b>	Surface boundary condition
	<b>trenxt</b>	Vertical diffusion (implicit method)
	<b>trcdia</b>	Time integration
	<b>trcdit</b>	Calls output routines
	<b>trcdid</b>	Writes tracer concentrations
	<b>trcdii</b>	Writes dynamical trends
	<b>trcdib</b>	Writes additional 2-D and 3-D diagnostics
	<b>trcwri</b>	Writes biological trends
		Writes restart file for passive tracers

### III-3 Parameters

*jptra* : number of tracers (2 by default).

*jpdiatrc* : number of dynamical trends (6 by default, 9 if *key\_trahdfeiv* is defined).

*jpdia2d* : number of additional 2-D arrays (user dependent).

*jpdia3d* : number of additional 3-D arrays (user dependent).

*jpdiabio* : number of biological trends (9 for NPZD, 15 for NNPZDDOM).

*jpkbio* : vertical level from which the demineralization model starts (user dependent).

### III-4 Namelist

There are two namelists. *Namelist.passivetr* is the general namelist for passive tracers. *Namelist.passivetr.sms* is the specific namelist for SMS terms.

#### 1. *Namelist.passivetr*

**NATTRC** : General information on tracers

*nwritetr* : time step frequency for tracer outputs

*lrsttr* : boolean. If true restarts the tracer module.

*nrsttr* : control of the restart time step.

*ctrcnm* : string for tracer short name

*ctrcnl* : string for tracer long name

*ctrcun* : string for tracer unit

*lutini* : boolean. If true initializes from a file

**NATNUM** : Numerics

*lhdf* : boolean . If true computes horizontal diffusion

*ndttrc* : passive tracer integration time step frequency

*rsc* : tuning coefficient for Smolarkiewicz scheme

*rtrn* : truncation value for Smolarkiewicz scheme

- **ncor** : number of corrective phases for Smolarkiewicz scheme
- **crosster** : boolean. If true computes crossterms for Smolarkiewicz scheme.
- **ahtrb0** : background eddy diffusivity for isopycnal diffusion (m<sup>2</sup>/s)

NATADD : Additional 2D-3D arrays for diagnostics

- **nwriteadd** : output frequency for additional 2D-3D arrays
- **ctrc3d** : short name for 3D arrays
- **ctrc3l** : long name for 3D arrays
- **ctrc3u** : units for 3D arrays
- **ctrc2d** : short name for 2D arrays
- **ctrc2l** : long name for 2D arrays
- **ctrc2u** : units for 2D arrays

NATRTD : Dynamical trends

- **nwritetrd** : output frequency for dynamical trends
- **luttrd** : boolean (one value per tracer). If true saves dynamical trends.

## 2. *Namelist.passivetracer.sms (example for the NPZD model)*

NATBIO : Biological parameters  
 NATOPT : Optical parameters  
 NATDBI: Biological trends

### III-5 Performances

Performances are calculated for a Smolarkiewicz scheme with one corrective loop, no cross terms, and a passive tracer time step four times that of the dynamical time step.

Domain	Code	Memory	CPU time per time step per grid point	Computer
ORCA2 182x152x31	OPA only with NNPZDDOM	580 Mb 800 Mb	0.45 x 10 <sup>-6</sup> s 0.67 x 10 <sup>-6</sup> s	NEC SX5

Academic 218x162x30	OPA only (no salinity)	384 Mb	$0.86 \times 10^{-6}$ s	Fujitsu VPP 300
	with NNPZDDOM	632 Mb	$1.27 \times 10^{-6}$ s	

The next table details performances for the off-line version of the model: Performances are computed for a Smolarkiewicz advection scheme with one corrective loop and with cross terms. Time step for tracers and transport is identical.

Domain	Code	Memory	CPU time per time step per grid point	Computer
ORCA2 182x152x31	HAMOCC3	602 Mb	$0.74 \times 10^{-6}$ s	Fujitsu VPP 5000
	P3ZD	782 Mb	$1.05 \times 10^{-6}$ s	
Academic 218x162x30	OPA only (no salinity)	384 Mb	$0.86 \times 10^{-6}$ s	Fujitsu VPP 300
	with NNPZDDOM	632 Mb	$1.27 \times 10^{-6}$ s	



## IV. SPECIFICITY OF THE *OFFLINE* CODE

### VI-1 Generalities

The passive tracer model is identical in on-line and off-line modes. When the off-line mode is set, the dynamical computations (OPA model) are replaced by an "off-line OPA" model. The off-line OPA model is a frame for the reading of the mask (meshmask file) and of previously computed dynamical fields. The off-line version of the tracer model is constructed with the *fait\_make\_offline* script.

### VI-2 Specific off-line options

*key\_off\_tra* : memory reservation and reading of temperature and salinity fields

*key\_off\_degrad* : model run with the degradation technique DEGINT. Isopycnal slopes and eddy induced velocities are read from a file instead of being computed. Additionally, this key activates some minor changes in the diffusion routines (trchdf.F and treczdf.F) required by DEGINT. For more information about DEGINT, the reader can refer to Aumont et al (1998). In the current version of the tracer model, this key can be activated only with the HAMOCC3 and P3ZD models.

### VI-3 Flow chart

Routines are sorted by call levels

Legend : *Standard OPA routines*      *Specific off-line OPA routines...* **Tracer routines.**

**Flow chart for the off-line code**

<b><u>Routine names</u></b>	<b><u>Details</u></b>
<i>modele</i>	Offline Ocean General Circulation Model
<b><i>opa</i></b>	initialization of parameters
<i>inipar</i>	constants
<i>parcst</i>	offline namelist read
<b><i>parlec</i></b>	control options
<i>parctl</i>	Initialisation for MPP
<i>inimpp</i>	read a meshmask file describing domain
<b><i>domrea</i></b>	prepares different time step for each level
<i>domstp</i>	Tracer model initialisation
<b><i>initrc</i></b>	Reads namelist.passivetr
<i>trclec</i>	Reads namelist for SMS
<i>trclsm</i>	Controls the coherence of options
<b><i>trcctl</i></b>	all fields are initialized to zero
<b><i>trcini</i></b>	initialization when restart: from trc.restart file
<b><i>trcrst</i></b>	initialization when no restart: analytic or from file
<b><i>trcdtr</i></b>	horizontal diffusion coefficient
<b><i>inihdf</i></b>	Dynamics
<b><i>dtadyn</i></b>	reads dynamics
<i>dynrea</i>	computes horizontal divergence
<i>div</i>	computes vertical velocity
<i>wzv</i>	computes equation of state
<i>eos</i>	computes Brunt-Vaisala frequency
<i>bn2</i>	computes isopycnal slope computation
<i>hdfslp</i>	task initialization
<i>mlbxinit</i>	call of tasks
<i>tskstart</i>	time step routine
<b><i>step</i></b>	dynamic and physic computing
<b><i>dtadyn</i></b>	passive tracer time step
<b><i>trcstp</i></b>	entry point for SMS routines
<b><i>trcsms</i></b>	Optics (example)
<i>trcopt</i>	Biology (example)
<i>trcbio</i>	Sedimentation (example)
<i>trcsed</i>	Horizontal advection (for Arakawa scheme)
<b><i>trchad</i></b>	Vertical advection (for Arakawa scheme)
<b><i>trczad</i></b>	3D advection (for Smolarkiewicz scheme)
<b><i>trc3ad</i></b>	Horizontal diffusion
<b><i>trchdf</i></b>	Surface boundary condition
<b><i>trcsbc</i></b>	Vertical diffusion (implicit method)
<b><i>trczdf</i></b>	Time integration
<b><i>trcnxt</i></b>	Calls output routines
<b><i>trcdia</i></b>	Writes tracer concentrations
<b><i>trcdit</i></b>	Writes dynamical trends
<b><i>trcdid</i></b>	Writes 2-D and 3-D diagnostics
<b><i>trcdii</i></b>	Writes biological trends
<b><i>trcdib</i></b>	Writes restart file for passive tracers
<b><i>trcwri</i></b>	waiting of tasks
<i>tskwait</i>	MPP specific end
<b><i>mppstop</i></b>	



## APPENDIX A : ADVECTION SCHEMES

### A-1 Arakawa and Smolarkiewicz advection schemes

The equation to be resolved in the advection of a tracer  $T$  within a velocity field  $U = (u, v, w)$ :

$$\frac{\partial T}{\partial t} + \frac{1}{b} \left[ \frac{\partial}{\partial i} (e_2 e_3 T u) + \frac{\partial}{\partial j} (e_1 e_3 T v) + \frac{\partial}{\partial k} (e_1 e_2 T w) \right] = 0 \quad (\text{A1})$$

where  $(i, j, k)$  is set of orthogonal curvilinear coordinates on the sphere, associated with the positively oriented orthogonal set of unit vector  $(\mathbf{i}, \mathbf{j}, \mathbf{k})$  linked to the earth such that  $\mathbf{k}$  is the local upward vector, and where  $(e_1, e_2, e_3)$  are the scale factors and  $b = e_1 e_2 e_3$ .

Equation (A-1) can be rewritten under the form:

$$\frac{\partial T}{\partial t} + \frac{1}{b} \sum_{m=1}^3 \frac{\partial}{\partial y_m} (A_m T) = 0 \quad (\text{A2})$$

$$\text{with the water mass fluxes } (A_1, A_2, A_3) = (e_2 e_3 u, e_1 e_3 v, e_1 e_2 w) \quad (\text{A3})$$

Given the values of a scalar  $q$  at two adjacent grid points, one can define the derivation and averaging at the in-between midpoint as:

$$\delta_i[q] = q(i + 1/2) - q(i - 1/2) \quad (\text{A4})$$

$$\bar{q}^i = \frac{1}{2} \{q(i + 1/2) + q(i - 1/2)\} \quad (\text{A5})$$

The positive and negative parts of  $q$  are defined at  $q$  points by:

$$\begin{aligned}
q^+ &= \frac{1}{2}(q + |q|) \\
q^- &= \frac{1}{2}(q - |q|)
\end{aligned}
\tag{A6}$$

The semi-discrete space equation for (A-3) corresponding to the second order spatial *Arakawa scheme* is:

$$\frac{\partial T}{\partial t} + \frac{I}{b_T} \left\{ \delta_i \left[ \bar{T}^{i+1/2} A_{1u} \right] + \delta_j \left[ \bar{T}^{j+1/2} A_{2v} \right] + \delta_k \left[ \bar{T}^{k+1/2} A_{3w} \right] \right\} = 0
\tag{A7}$$

where  $b_T = e_{1T} e_{2T} e_{3T}$  is the grid volume at T point.

The *upwind scheme* advects the tracer as a function of the direction of the flow, and corresponds to a different semi-discrete space equation for (A-3) :

$$\begin{aligned}
\frac{\partial T}{\partial t} + \frac{I}{b_T} \left\{ \delta_i \left[ \left( T^i A_{1u}^+ + T^{i+1} A_{1u}^- \right) \right] + \delta_j \left[ \left( T^j A_{2v}^+ + T^{j+1} A_{2v}^- \right) \right] \right. \\
\left. + \delta_k \left[ \left( T^k A_{3w}^+ + T^{k+1} A_{3w}^- \right) \right] \right\} = 0
\end{aligned}
\tag{A8}$$

There is an implicit diffusion inherent to the upwind scheme that can be easily computed. Indeed, the development to the second order of (A-8) in space and time, in the hypothesis of a time constant mass flux, leads to, after substitution in (A-8):

$$\frac{\partial T}{\partial t} + \frac{1}{b} \sum_{m=1}^3 \frac{\partial}{\partial y_m} (A_m T) + \frac{1}{b} \sum_{m=1}^3 \frac{\partial}{\partial y_m} (A_m^{(1)} T) = 0
\tag{A9}$$

where the expression of the ‘‘implicit mass flux’’ at this order is :

$$A_m^{(1)} = \frac{1}{T} \left( A_m \frac{\Delta t}{2} \sum_{n \neq m} \frac{A_n}{b} \frac{\partial T}{\partial y_n} + \frac{\Delta t}{2} \frac{A_m^2}{b} \frac{\partial T}{\partial y_m} - \frac{|A_m|}{2} \frac{\partial T}{\partial y_m} \right)
\tag{A10}$$

The principle of the FCT method is to advect the tracer using an upwind scheme, then compute the  $A_m^{(1)}$  term from the mass flux and the new tracer concentration, and finally to advect these new concentrations with another upwind but opposite mass fluxes  $-A_m^{(1)}$ . The index (1) refers to the number of the correcting phase. The method therefore consists in correcting the upwind scheme with an anti-diffusive term that works against the implicit diffusion.

The discrete form of these mass fluxes is:

$$\begin{aligned}
A_{1u}^{(1)} &= \frac{1}{\bar{T}^{i+1/2}} \left\{ \frac{\Delta t}{2} \frac{A_{1u}}{b_u} \left( \overline{\left( \delta_{j+1/2} [T] A_{2v} \right)^{i+1/2, j}} + \overline{\left( \delta_{k+1/2} [T] A_{2v} \right)^{i+1/2, k}} \right) \right. \\
&\quad \left. + \frac{\Delta t}{2} \frac{A_{1u}^2}{b_u} \delta_{i+1/2} [T] - \frac{|A_{1u}|}{2} \delta_{i+1/2} [T] \right\}
\end{aligned}
\tag{A11}$$

with similar expressions for  $A_{2v}^{(1)}$  and  $A_{3w}^{(1)*}$ .

The second upwind is done by replacing  $A$  by  $-A^{(1)}$  in (A-8), by advecting the field  $T^{(1)}$  obtained after the first upwind, and temporally integrated at the first order by replacing the temporal derivative in (A-8) by:

$$\frac{\partial T}{\partial t} = \frac{T^{(1)} - T}{\Delta t} \quad (\text{A12})$$

There are different options in the FCT method:

- the cross-terms in (A-11) can be neglected (terms that have the form  $A_n A_m$ ,  $n \neq m$ ,  $i$ . the first term in the left hand side of (A-10))
- corrective fluxes  $-A^{(1)}$  can be multiplied by a scale factor larger than 1.
- the corrective phase can be repeated as many times as needed (by calculating  $A^{(2)}$ , and advecting by a new upwind, and so on), the implicit diffusion of the scheme being diminished by each repetition.

## A-2 Associated temporal schemes

The time differencing scheme used in OPA for the advection of active tracers is the centered leapfrog scheme:

$$T(t + \Delta t) = T(t - \Delta t) + 2\Delta t F[T(t), U(t)] \quad (\text{A13})$$

This scheme is used together with a Robert-Asselin filter to integrate in time an advective transport spatially discretized following the Arakawa scheme.

The scheme is of second order in space and time; however the time filter degrades the time accuracy from second to first order.

The FCT method requires by construction a forward time scheme:

$$T(t + \Delta t) = T(t) + \Delta t F[T(t), U(t)] \quad (\text{A14})$$

This scheme can be unstable for active tracers, but become stable when velocities are centered in time:

---

\* The  $k$ -axis is oriented downward in the code, and upward in the equations. This leads to a different sign in the code for the second and third terms of  $A_{3w}^{(1)}$ .

$$T(t + \Delta t) = T(t - \Delta t) + 2\Delta t F[T(t - \Delta t), U(t)] \quad (\text{A15})$$

The integration is therefore done over a doubled time step (which implies that  $\Delta t$  must be replaced by  $2\Delta t$  in (A-10), (A-11) et (A-12), and tracers are transported with the velocity field calculated in between these two time steps).

### A-3 Numerical cost

The cost of the Arakawa scheme is relatively low. However, in order to insure the stability of the scheme, it is necessary to explicitly add spatial and temporal diffusion, which can greatly increase the overall cost.

The FCT scheme is much more time consuming than the Arakawa scheme, although its cost strongly depends on the number of corrective phases, the computation or not of cross-terms, and the time step. Furthermore, in eddy-resolving configurations, it can be used without additional lateral diffusion.

## APPENDIX B : THE NPZD BIOGEOCHEMICAL MODEL

The NPZD model consists of four prognostic variables expressed in terms of their nitrogen content: nutrients (N), phytoplankton (P), zooplankton (Z) and detritus (D).

### B-1 The surface layer NPZD model

Within the first *jpbio* levels, the biogeochemical Source Minus Sink terms for each of the variables are (with model parameters in Table B1):

$$S(N) = -\square_p L_l L_N P + \square_z Z + \square_d D \quad (\text{B1})$$

$$S(P) = \square_p L_l L_N P - G_p - m_p P \quad (\text{B2})$$

$$S(Z) = a_p G_p + a_d G_d - \square_z Z - m_z Z \quad (\text{B3})$$

$$S(D) = (1 - a_p) G_p + (1 - a_d) G_d + m_p P + m_z Z - \square_d D - G_z^d - V_d \partial_z D \quad (\text{B4})$$

The formulation for phytoplankton growth (*i.e.* primary production,  $\square_p L_l L_N P$ ) takes into account nutrient and light limitations. Nutrient limitation has the Michaelis-Menten kinetics:

$$L_N = \frac{N}{N + K_N} \quad (\text{B5})$$

Light limitation has the Webb *et al.* (1974) type

$$L_l = 1 - e^{-PAR/K_{PAR}} \quad (\text{B6})$$

Grazing of phytoplankton and detritus is formulated following Fasham *et al.* (1990):

$$G_p = g_z Z \frac{P^2}{(P + D)K_z + P^2 + D^2} \quad (\text{B7})$$

$$G_d = g_z Z \frac{D^2}{(P + D)K_z + P^2 + D^2} \quad (\text{B8})$$

The other biogeochemical interactions taken into account are phytoplankton mortality, zooplankton mortality and zooplankton excretion (these last two processes are inhibited when zooplankton concentration is below a given threshold), fecal pellet production, detritus sedimentation and detritus remineralization.

*Table B1. Parameters for the NPZD model*

Nutrient half-saturation constant	$K_n$	0.5	mmole/m <sup>3</sup>
Phytoplankton maximal growth rate	$\square_p$	2	d <sup>-1</sup>
Carbon/Chlorophyll ratio	$R_{c-chl}$	55	gC/gChl
Half-saturation constant for light	$K_{PAR}$	33.33	W/m <sup>2</sup>
Phytoplankton mortality rate	$m_p$	0.03	d <sup>-1</sup>
Zooplankton maximal grazing rate	$g_z$	0.75	d <sup>-1</sup>
Half-saturation constant for grazing	$K_z$	1	mmole/m <sup>3</sup>
Assimilated fraction of phytoplankton	$a_p$	0.7	
Assimilated fraction of detritus	$a_d$	0.5	
Zooplankton excretion rate	$\square_z$	0.1	d <sup>-1</sup>
Zooplankton mortality rate	$m_z$	0.03	d <sup>-1</sup>
Detritus sedimentation speed	$V_d$	5	m d <sup>-1</sup>
Detritus remineralization rate	$\square_d$	0.09	d <sup>-1</sup>

## B-2 The optical model

The photosynthetic available radiation (*PAR*) is derived from a light absorption model. Only a fraction of the light field (43%) can be used for photosynthesis. Two different light wavelengths are considered (Table B2). The absorption coefficients depend on the local phytoplankton concentrations:

$$\lambda_r = \lambda_{r0} + \lambda_{rp} Chl^l \quad (\text{B9})$$

$$\lambda_g = \lambda_{g0} + \lambda_{gp} Chl^{l_g} \quad (B10)$$

$$Chl = 12 P R_{c:n} / R_{pig} R_{c:chl} \quad (B11)$$

$$PAR_g = PAR_g(z - \Delta z) \left(1 - e^{-\lambda_g \Delta z}\right) \quad (B12)$$

$$PAR_r = PAR_r(z - \Delta z) \left(1 - e^{-\lambda_r \Delta z}\right) \quad (B13)$$

$$PAR(z) = PAR_r(z) + PAR_g(z) \quad (B14)$$

As phytoplankton concentrations are homogeneous over a  $T$ -level, absorption coefficients are constant over these levels. The absorption equations B12 and B13 can therefore be recursively solved from the upper to the lower  $W$ -level, starting from the surface, *i.e.* omitting the reference to the wavelength:

$$PAR_w(k) = PAR_w(k-1) \left(1 - e^{-\lambda(k-1)e_{3T}(k-1)}\right) \quad (B15)$$

$$PAR_w(1) = PAR_r(z=0) \text{ ou } PAR_g(z=0) \quad (B16)$$

Then the averaged value of PAR at the  $T$ -level ( $PAR_T(k)$ ) is calculated as the averaged integral value of PAR over the  $T$ -level:

$$PAR_T(k) = \frac{PAR_w(k-1)}{\lambda(k)e_{3T}(k)} \left(1 - e^{-\lambda(k)e_{3T}(k)}\right) \quad (B17)$$

Table B2. Parameters for the optical model

Water absorption in red	$\lambda_{r0}$	0.225	$m^{-1}$
Water absorption in blue	$\lambda_{g0}$	0.0232	$m^{-1}$
Pigments absorption in red	$\lambda_{rp}$	0.037	$m^{-1} (mg Chl / m^3)^{-l_r}$
Pigments absorption in blue	$\lambda_{gp}$	0.074	$m^{-1} (mg Chl / m^3)^{-l_g}$
Power law for absorption in red	$l_r$	0.629	
Power law for absorption in blue	$l_g$	0.674	
Contribution of Chlorophyll to absorbing pigments	$R_{pig}$	0.7	
C:N Redfield ratio	$R_{c:N}$	7	$mg C / mg Chl$
C:Chl ratio	$R_{c:Chl}$	55	$mg C / mg Chl$

### B-3 Remineralization

Below the vertical level  $jpkbio$ , remineralization processes are preponderant and the surface model does not apply. Remineralization below the surface layer is simply parameterized by a decay of phytoplankton, zooplankton and detritus in nutrients. This parameterization enables conservation of total nitrogen.

$$S(N) = \tau_r(P + Z + D) \quad (B18)$$

$$S(Z) = -\tau_r Z \quad (B19)$$

$$S(P) = -\tau_r P \quad (B20)$$

$$S(D) = -\tau_r D - V_d \partial_z D \quad (B21)$$

The decay rate  $\tau_r$  varies linearly with depth, between prescribed minimal and maximal values.



## APPENDIX C : THE NNPZDDOM BIOGEOCHEMICAL MODEL

The NNPZDDOM model consists of six prognostic variables expressed in terms of their nitrogen content: nitrate, ammonium, phytoplankton, zooplankton, detritus and dissolved organic matter.

### C-1 The surface layer NNPZDDOM model

Within the first *jpbio* levels, the biogeochemical Source Minus Sink terms for each of the variables are (with model parameters in Table C1):

$$S(NO_3) = -\square_p L_I L_{NO_3} P + \square_n NH_4 \quad (C1)$$

$$S(NH_4) = -\square_p L_I L_{NH_4} P + f_n \left( \gamma \square_p L_I (L_{NO_3} + L_{NH_4}) P + \square_z Z + \square_d D \right) - \square_n NH_4 \quad (C2)$$

$$S(P) = (1 - \gamma) \square_p L_I (L_{NO_3} + L_{NH_4}) P - G_p - m_p P \quad (C3)$$

$$S(Z) = a_p (G_p + G_d) - m_z Z^2 - \square_z Z \quad (C4)$$

$$S(D) = (1 - a_p) (G_p + G_d) + m_p P - G_d - \square_d D - V_d \partial_z D \quad (C5)$$

$$S(DOM) = (1 - f_n) \left( \gamma \square_p L_I (L_{NO_3} + L_{NH_4}) P + \square_z Z + \square_d D \right) - \square_{dom} DOM \quad (C6)$$

The formulation for phytoplankton growth takes into account limitation by both nutrients and light. Nutrient limitation follows the Hurt and Armstrong (1996) kinetics:

$$L_{NH_4} = \frac{NH_4}{NH_4 + K_N} \quad (C7)$$

$$L_{NO_3} = \frac{K_N * NO_3}{(NH_4 + K_N)(NO_3 + NH_4 + K_N)} \quad (C8)$$

Light limitation follows Webb *et al.* (1974)

$$L_l = 1 - e^{-PAR/K_{PAR}} \quad (C9)$$

Grazing of phytoplankton and detritus is formulated following Fasham *et al.* (1990):

$$G_p = g_z Z \frac{P^2}{(P + D)K_z + P^2 + D^2} \quad (C10)$$

$$G_d = g_z Z \frac{D^2}{(P + D)K_z + P^2 + D^2} \quad (C11)$$

Other modeled biogeochemical interactions include phytoplankton mortality, zooplankton mortality (that is not reinjected in the surface layer but is remineralized below), zooplankton excretion, fecal pellet production, detritus sedimentation, detritus remineralization, nitrification, and dissolved organic matter break down.

Table C1. Parameters for the NNPZDDOM model

Nutrient half-saturation constant	$K_n$	0.1	mmole/m <sup>3</sup>
Phytoplankton maximal growth rate	$\square_p$	1/0.5	d-1
Carbon/Chlorophyll ratio	$R_{c-chl}$	60	gC/gChl
Half-saturation constant for light	$K_{PAR}$	33.33	W/m <sup>2</sup>
Phytoplankton exudation	$\gamma$	0.05	
Phytoplankton mortality rate	$m_p$	1/20	d-1
Zooplankton maximal grazing rate	$g_z$	1/1	d-1
Half-saturation constant for grazing	$K_z$	1	mmole/m <sup>3</sup>
Assimilated fraction of phytoplankton	$a_p$	0.7	
Assimilated fraction of detritus	$a_d$	0.5	
Zooplankton excretion rate	$\square_z$	1/10	d-1
Zooplankton mortality rate	$m_z$	1	mmoleN/m <sup>3</sup> d-1
Nitrification rate	$\square_n$	1/20	d-1
DOM breakdown rate	$\square_{dom}$	1/30	d-1
DOM/NH <sub>4</sub> excretion ratio	$f_n$	0.75	
Detritus sedimentation speed	$V_d$	5	m d-1
Detritus remineralization rate	$\square_d$	1/20	d-1

## C-2 The optical model

The optical model is the same as for the NPZD model (see Appendix B-2).

## C-3 Remineralization

Below the vertical level  $z_{bio}$  (corresponding to the depth  $z_{bio}$ ), remineralization processes are preponderant and the surface model does not apply. A decay of phytoplankton, zooplankton and detritus in nutrients, and a local (i.e. on the same vertical) redistribution of zooplankton mortality according to Martin's profile parameterize remineralization below the surface layer. This parameterization allows conservation of total nitrogen.

$$S(NO_3) = \tau_r(NH_4 + P + Z + D + DOM) + \partial_z f \quad (C21)$$

$$S(NH_4) = -\tau_r NH_4 \quad (C22)$$

$$S(P) = -\tau_r P \quad (C23)$$

$$S(Z) = -\tau_r Z \quad (C24)$$

$$S(D) = -\tau_r D - V_d \partial_z D \quad (C25)$$

$$S(DOM) = -\tau_r DOM \quad (C26)$$

The decay rate  $\tau_r$  equals 1/20days.

The remineralization flux  $f$  is defined as:

$$f(z_{bio}) = \int_0^{z_{bio}} m_z Z^2 dz \quad (C27)$$

$$f(z) = f(z_{bio}) \left( z/z_{bio} \right)^{-0.858} \quad (C28)$$

We add a condition for no deposition on the ocean floor:

$$f(z_{bottom}) = 0. \quad (C29)$$



## APPENDIX D : THE HAMOCC3 BIOCHEMICAL MODEL

The biogeochemical model HAMOCC3 (Maier-Reimer, 1993) is coupled to OPA. This model includes seven prognostic tracers necessary for the computation of the different biogenic fluxes of carbon: dissolved inorganic carbon (DIC), alkalinity, O<sub>2</sub>, calcite, PO<sub>4</sub><sup>3-</sup>, particulate organic carbon (POC), and dissolved silicate.

### D-1 The surface layer biological production

These fluxes are divided into two components; the soft tissue pump and the hard tissue counterpump. The soft tissue pump is reduced, in the model, to the export production (EP), defined simply as the part of the primary production transported out of the euphotic zone. EP is computed as

$$EP = r_0 \frac{50m}{Z_m} \frac{T + 2}{T + 10} \frac{PO_4^{3-}}{PO_4^{3-} + P_0} PO_4^{3-} \quad (D1)$$

where  $r_0$  is the maximum productivity rate,  $I$  is a normalized light factor,  $Z_m$  is the mixed layer depth,  $T$  is temperature (degrees Celsius), and  $P_0$  is a half saturation constant. Export production in nutrient-poor water is reduced by a simple Michaelis-Menten kinetics formula that depends on the local concentration of PO<sub>4</sub><sup>3-</sup>. In HAMOCC3, PO<sub>4</sub><sup>3-</sup> is chosen as the limiting nutrient to avoid complexities associated with nitrogen cycling. The thickness of the euphotic zone is set to 50 m globally. The light factor  $I$  is defined as the integration of the cosine of the solar angle over the day length, normalized to be comprised between 0 and 1. Cloud cover is ignored in this computation. The maximum production efficiency  $r_0$  was chosen by Maier-Reimer (1993) to adjust his model output to fit the observed surface phosphate distribution.

The intensities of the hard tissue counterpump and of the silicate pump are deduced from export production. Two potential production functions are defined for calcite and silicate:

$$PSi = \min(Si, 600EP) \frac{Si}{Si + Si_0} \quad (D2)$$

$$PCaCO_3 = \left( \frac{CaCO_3}{C} \right)_{\max} R_{C/P} \frac{e^{0.1(T-10)}}{1 + e^{0.1(T-10)}} EP \quad (D3)$$

The temperature dependent function for calcite production ensures a reduction of this production in cold waters as shown by the observations. From these two potential functions, actual production for both silicate and calcite can be defined:

$$Pr Si = PSi \frac{PSi}{PSi + PCaCO_3} \quad (D4)$$

$$Pr CaCO_3 = PCaCO_3 \frac{Si}{PSi + Si_0} \quad (D5)$$

## D-2 Export and Remineralization

POC produced in the euphotic zone is exported instantaneously below 100 m. The vertical profile of the POC flux is described according to a power law function (Berger *et al.*, 1987):

$$F(POC) = EP \left( \frac{100m}{z} \right)^{0.8} \quad (D6)$$

Remineralization of POC below the productive zone is simply parameterized in HAMOCC3 by a decay of POC:

$$S(POC) = -\tau_r POC \quad (D7)$$

The decay rate depends on temperature:

$$\tau_r = b_0 + b_1(T + 2) \quad (D8)$$

Remineralization rate of organic matter increases with temperature.  $b_0$  is set to 0 everywhere except in the deepest box of the water column to simulate enhanced degradation of organic matter due to benthic organisms.

In HAMOCC3, denitrification is not considered. Thus the remineralization of the organic matter is restricted to regions with sufficient oxygen ( $> 1 \text{ } \mu\text{mol/L}$ ). Otherwise, POC is preserved and transported by advection and diffusion.

Exponential functions are prescribed to predict the export of calcareous shells and opal:

$$F(Si) = Pr Si e^{-z/z_{Si}} \quad (D9)$$

$$F(CaCO_3) = Pr CaCO_3 e^{-z/z_{CaCO_3}} \quad (D10)$$

Silicate is instantaneously remineralized within the ocean.

Calcite dissolves with respect to the degree of saturation of seawater. The saturation degree in calcite of seawater is computed in the model assuming that  $[Ca^{2+}]$  is constant in the ocean.

$$S(CaCO_3) = -\frac{I - \Delta CO_3}{CO_{3,0} + |\Delta CO_3|} CaCO_3 \quad (D11)$$

where  $\Delta CO_3$  is the deviation of  $CO_3^{2-}$  from saturation:

$$\Delta CO_3 = CO_3^{2-} - \frac{k_{CO_3}}{Ca^{2+}} \quad (D12)$$

Thus, dissolution rate of calcite increases when saturation decreases. With the constants chosen in the model (see Table D1), for a saturation of  $-20 \text{ } \mu\text{mol/L}$ , 83% of calcite dissolves each month. For a saturation of  $20 \text{ } \mu\text{mol/L}$ , this proportion drops to 22%.

### D-3 Gas exchange

At the sea surface, the ocean exchanges  $CO_2$  and  $O_2$  with the atmosphere. The net flux from air to sea  $F$  is proportional to the difference between the partial pressure of the gas in air  $P_a$  and that in surface seawater  $P_s$ :

$$F = k \alpha (P_a - P_s) \quad (D13)$$

where  $k$  is the gas transfer velocity (in m/s),  $\alpha$  is the gas solubility ( $\text{mol}\cdot\text{m}^{-3}\cdot\text{atm}^{-1}$ ). The piston velocity of  $CO_2$  is computed by using equation (D8) from Wanninkhof (1992), a quadratic function of wind speed that includes a chemical enhancement at low wind speeds. We used a climatology of the monthly mean wind speeds and variances (Boutin *et al.*, 1997) derived from special sensor microwave images (SSM/I) wind speeds. The resulting gas

exchange coefficient  $K$  ( $K=k\alpha$ ) for  $\text{CO}_2$  has been scaled so that its global mean value equals  $0.061 \text{ mol.m}^{-2}.\text{matm}^{-1}.\text{yr}^{-1}$  deduced from  $^{14}\text{C}$  observations Broecker *et al.* (1985). The piston velocity of  $\text{O}_2$  is computed according to the formulation from Liss and Merlivat (1986).

*Table D1. Parameters for the HAMOCC3 model*

Nutrient half-saturation constant	$P_0$	0.004	$\square$ mol/L
Production efficiency	$r_0$	0.25	month <sup>-1</sup>
Silicate half-saturation constant	$\text{Si}_0$	4	$\square$ mol/L
Maximum rain ratio	$(\text{C}/\text{CaCO}_3)_{\text{max}}$	0.35	
Silicate export length	$z_{\text{Si}}$	1000	m
Calcite export length	$z_{\text{CaCO}_3}$	12000	m
First remineralization constant	$b_0$	1/6	month <sup>-1</sup>
Second remineralization constant	$b_1$	0.002	month.(°C) <sup>-1</sup>
Calcium concentration	$\text{Ca}^{2+}$	0.103	$\square$ mol/L
Calcite half-saturation constant	$\text{CO}_{3,0}$	10	$\square$ mol/L



## APPENDIX E : THE P3ZD BIOCHEMICAL MODEL

The P3ZD includes five prognostic variables required to compute the biological processes: phytoplankton, POM,  $PO_4^3$ , zooplankton, and DOM. All the variables except phosphate are expressed in carbon. The model includes four additional variables to describe the carbon cycle and the silicon cycle: DIC, alkalinity, calcite, oxygen and silicate.

### E-1 The surface layer P3ZD model

Within the first *jpbio* levels (generally set to 10), the biogeochemical Source Minus Sink terms for each of the variables are (with model parameters in Table E1):

$$S(PO_4) = R_{P/C} \left( -\square_p L_M L_I L_{PO_4} P + \varepsilon m_z \frac{Z^2}{K_z^1 + Z} + \square_{dom} DOM \right) \quad (E1)$$

$$S(P) = (1 - \gamma) \square_p L_M L_I L_{PO_4} P - G_p - m_p \frac{P}{K_p + P} - w_p P^2 \quad (E2)$$

$$S(Z) = a_z (G_p + G_d) - m_z \frac{Z^2}{K_z^1 + Z} - \square_z \frac{Z^2}{K_z^2 + Z} \quad (E3)$$

$$S(D) = (1 - a_z) (G_p + G_d) + m_p \frac{P}{K_p + P} + w_p P^2 \quad (E4)$$

$$+ (1 - \varepsilon) m_z \frac{Z^2}{K_z^1 + Z} - G_d - \square_d D - V_d \partial_z D$$

$$S(DOM) = \gamma \square_p L_M L_l L_{PO_4} P + \square_z \frac{Z^2}{K_z^2 + Z} + \square_d D - \square_{dom} \frac{PO_4}{K_{dom}^1 + PO_4} \frac{DOM}{K_{dom}^2 + DOM} DOM \quad (E5)$$

The formulation for phytoplankton growth takes into account limitation by both phosphate and light. Nutrient limitation follows a simple Michaelis-Menten dynamics:

$$L_{NH_4} = \frac{PO_4}{PO_4 + K_N} \quad (E6)$$

Light limitation follows Webb *et al.* (1974) with a photo-inhibition term

$$L_l = \left(1 - e^{-\alpha PAR / \square_p}\right) e^{\beta PAR / \square_p} \quad (E7)$$

Furthermore, equation for phytoplankton growth includes an additional limitation factor that describes the effect of mixing following Andre (1990) formulation

$$\begin{aligned} L_M &= 1 & \text{if} & \quad Z_e > Z_m \\ L_M &= 0.5 & \text{if} & \quad Z_m > 2Z_e \\ L_M &= \left(1 - 0.5 \frac{Z_m}{Z_e}\right) & \text{if} & \quad Z_e < Z_m < 2Z_m \end{aligned} \quad (E8)$$

Grazing of phytoplankton and detritus by zooplankton is formulated following Fasham *et al.* (1990):

$$G_p = g_z Z \frac{a_p P}{K_z + a_p P + a_d D} \quad (E10)$$

$$G_d = g_d Z \frac{a_d D}{K_z + a_p P + a_d D} \quad (E11)$$

where both variables are defined according to the following equations:

$$a_p = \frac{x_p P}{x_p P + x_d D} \quad (E12)$$

$$a_d = \frac{x_d D}{x_p P + x_d D} \quad (E13)$$

The preferences of zooplankton for detritus and phytoplankton are given in the parameter table E1.

Table E1. Parameters for the P3ZD model

Nutrient half-saturation constant	$K_n$	0.05	mmol P/m <sup>3</sup>
Phytoplankton growth rate	$\mu$	0.6	d <sup>-1</sup>
Initial P-I slope	$\alpha$	0.05	d/(W/m <sup>2</sup> )
Photo-inhibition parameter	$\beta$	0.02	d/(W/m <sup>2</sup> )
Phytoplankton exudation	$\gamma$	0.05	d <sup>-1</sup>
Phytoplankton mortality rate	$m_p$	0.05	d <sup>-1</sup>
Half-saturation constant for Phyto. mortality	$K_p$	1	mmol C/m <sup>3</sup>
Phytoplankton quadratic loss term	$w_p$	0.013	mmol C/m <sup>3</sup> /d
Zooplankton maximal grazing rate	$g_z$	0.8	d <sup>-1</sup>
Half-saturation constant for grazing	$K_z$	7.6	mmole C/m <sup>3</sup>
Preference for phytoplankton	$X_p$	0.8	
Preference for detritus	$X_d$	0.2	
Assimilated fraction of phytoplankton	$a_z$	0.7	
Zooplankton excretion rate	$\mu_z$	0.05	d <sup>-1</sup>
Zooplankton mortality rate	$m_z$	0.1	d <sup>-1</sup>
Half-saturation constant for zoo mortality	$K_z^1$	1	mmole C/m <sup>3</sup>
Half-saturation constant for zoo excretion	$K_z^2$	1	mmole C/m <sup>3</sup>
DOM breakdown rate	$\mu_{dom}$	1/30	d <sup>-1</sup>
DOM first-saturation constant	$K_{dom}^1$	15	mmole C/m <sup>3</sup>
DOM second half-saturation constant	$K_{dom}^2$	0.3	mmole P/m <sup>3</sup>
Detritus sedimentation speed	$V_d$	5	m d <sup>-1</sup>
Detritus remineralization rate	$\mu_d$	1/20	d <sup>-1</sup>

## E-2 The optical model

The photosynthetic available radiation (*PAR*) is derived from a light absorption model. Only a fraction of the light field (45%) can be used for photosynthesis. Two different light wavelengths are considered (Table B2). The absorption coefficients depend on the local phytoplankton concentrations:

$$\lambda_r = \lambda_{r0} + \lambda_c \text{ Chl} \quad (\text{E14})$$

$$\lambda_g = \lambda_{g0} + \lambda_c \text{ Chl} \quad (\text{E15})$$

$$PAR_g(z=0) = PAR_r(z=0) = 0.45 Q_{sol} / 2 \quad (E16)$$

$$PAR_g(z) = PAR_g(z - \Delta z) \left(1 - e^{-\lambda_g \Delta z}\right) \quad (E17)$$

$$PAR_r(z) = PAR_r(z - \Delta z) \left(1 - e^{-\lambda_{rg} \Delta z}\right) \quad (E18)$$

$$PAR(z) = PAR_r(z) + PAR_g(z) \quad (E19)$$

As phytoplankton concentrations are homogeneous over a  $T$ -level, absorption coefficients are constant over these levels. Numerical embedding of the optical model is done the same way as for the NPZD model (see Appendix B). In this model, phytoplankton is supposed to mix rapidly in the mixed layer relative to its growth rate and photoadaptation to local conditions of light. Thus, the PAR is averaged over the whole mixed layer.

Chlorophyll is diagnostically diagnosed from phytoplankton following Doney et al (1996) formulation:

$$Chl/C = \frac{PO4}{K_N + PO4} \left( (Chl/C)_{max} - (Chl/C)_{min} \min\left(1, \frac{PAR}{PAR_0}\right) \right) \quad (E20)$$

Table E2. Parameters for the optical model

Water absorption in red	$\lambda_{r0}$	0.4	$m^{-1}$
Water absorption in blue	$\lambda_{g0}$	0.027	$m^{-1}$
Pigments absorption	$\lambda_c$	0.016	$m^{-1}(mg\ Chl/m^3)$
Minimum Chl/C	$(Chl/C)_{min}$	0.2	$mg\ Chl/m^3$
Maximum Chl/C	$(Chl/C)_{max}$	0.33	$mg\ Chl/m^3$
Critical PAR for Chl/C	$PAR_0$	90	$W/m^2$

### E-3 Remineralization

Below the vertical level  $jpbio$  (corresponding to the depth  $z_{bio}$ ), remineralization processes are preponderant. The same model applies except that phytoplankton growth is set to 0. The particulate organic matter that sinks below the depth  $z_{bio}$  is instantaneously exported in the water column according to Martin's profile (see Appendix D, equation D6). There is no sedimentation deposition on the sea floor. Thus, the POM flux at the sea floor is set to 0.

In the P3ZD model, denitrification is considered. When oxygen falls below a critical level ( $< 1 \text{ } \mu\text{mol/L}$ ), remineralization of organic matter is still ongoing but without any oxygen consumption.

#### E-4 Carbon and silicon cycles

Production of calcareous shells by phytoplankton is described by the following equation:

$$\text{Pr } CaCO_3 = \frac{CaCO_3}{C} \frac{P + Z}{\int_0^{z_{bio}} (P + Z) dz} EP \quad (\text{E21})$$

where EP is the amount of POM that sinks below the depth  $z_{bio}$ .

Computation of the rain-ratio ( $CaCO_3/C$ ) is the same as in the HAMOCC3 model (see equation D3 in Appendix D). The calcite produced in the upper column is then exported instantaneously below  $z_{bio}$  according to the same exponential law as in the HAMOCC3 model (see equation D10). Dissolution of calcite follows equation D11.

Biogenic silicate production is describing according to:

$$\text{Pr } Si = \left( \frac{Si}{C} \right) \left( (1 - a_z)(G_p + G_d) + m_p \frac{P^2}{K_p + P} + w_p P^2 \right) \frac{Si}{K_{Si}^1 + Si} \quad (\text{E22})$$

where

$$\frac{Si}{C} = \left( \frac{Si}{C} \right)_{\max} \frac{Si}{K_{Si}^2 + Si} \frac{I}{1 + e^{0.1(T-10)}} \quad (\text{E23})$$

Biogenic silicate is then instantaneously exported below  $z_{bio}$  as in the HAMOCC3 model (see equation D9).

Table E3. Parameters for the carbon and silicon model

Maximum ( $CaCO_3/C$ )	$(CaCO_3/C)_{\max}$	0.13	
Maximum ( $Si/C$ )	$(Si/C)_{\max}$	0.45	
First half-saturation constant for silicate	$K_{Si}^1$	2	mmole Si/m <sup>3</sup>
Second half-saturation constant for silicate	$K_{Si}^2$	4	mmole Si/m <sup>3</sup>